1-Azacyclononan-2-one

Other names:	1H-Azonin-2(3H)-one, hexahydro-
	2-Perhydroazoninone
	2-azacyclononanone
	2H-Azonin-2-one, octahydro-
	8-Aminooctanoic acid lactam
	8-Octanelactam
	Azacyclononan-2-one
	Caprylactam
	Caprylolactam
	NSC 59017
	Octahydro-2H-azonin-2-one
	Octamethylenimine, 2-oxo-
	Octanoic acid, 8-amino-, lactam
	cyclooctanone isooxime
	«eta»-Caprylactam
	«omega»-Caprylolactam
	«omega»-Octalactam
Inchi:	InChI=1S/C8H15NO/c10-8-6-4-2-1-3-5-7-9-8/h1-7H2,(H,9,10)
InchiKey:	YDLSUFFXJYEVHW-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	O=C1CCCCCCCN1
Mol. weight [g/mol]:	141.21
CAS:	935-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-22.54	kJ/mol	Joback Method
hf	-252.16	kJ/mol	Joback Method
hfus	10.04	kJ/mol	Joback Method
hvap	45.66	kJ/mol	Joback Method
ie	9.12	eV	NIST Webbook
log10ws	-2.03		Crippen Method
logp	1.457		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
tb	535.84	K	Joback Method
tc	789.05	K	Joback Method

tf	354.23	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.80	J/mol×K	535.84	Joback Method
cpg	311.06	J/mol×K	578.04	Joback Method
cpg	330.25	J/mol×K	620.24	Joback Method
cpg	348.31	J/mol×K	662.45	Joback Method
cpg	365.20	J/mol×K	704.65	Joback Method
cpg	380.86	J/mol×K	746.85	Joback Method
cpg	395.24	J/mol×K	789.05	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C935308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of reaction of lanthanide trifluoroacetate trihydrate with 2-azacyclononanone to form lanthanide trifluoroacetate-tris 2-azacyclononanone:	https://www.doi.org/10.1016/j.tca.2006.12.017

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume